EXOMOLHD: PHOTODISSOCIATION OF DIATOMIC MOLECULES

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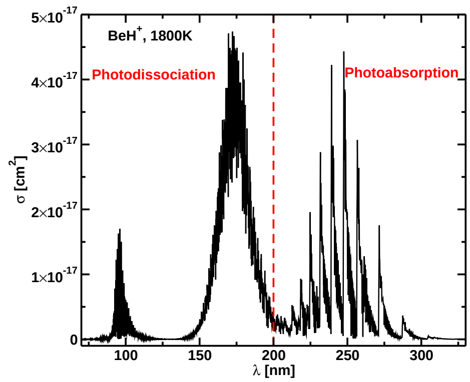

The destruction of molecules by photodissociation influences the composition and dynamics of exoplanets, particularly in the presence of a UV-rich stellar environments, where molecules are hot. Current photodissociation calculations generally assume $T = 0$ K, appropriate for the cold interstellar medium but inadequate for hot (exo)planets and stars. We compute temperature-dependent photodissociation cross sections for molecules found in these atmospheres. The cross sections are calculated by solving the nuclear-motion Schrödinger equation as part of the ExoMol project using codes Duo and Exocross[a], and averaging results obtained as discrete spectra. We benchmark our results for three systems. The general validity of the methodology is tested considering the $A^1\Pi \leftarrow X^1\Sigma^+$ transition of HCl at low T. Our cross sections and rates agree with published results[b] ($2.31*10^{-10}$ s^{-1} versus $2.10*10^{-10}$ s^{-1} respectively). We also reproduce calculated photodissociation cross section of BeH^+ at T=1800 K.[c] We performed the simulations considering the three excited states, $A^1\Sigma^+$, $B^1\Pi$ and $C^1\Sigma^+$, see figure. The photodissociation spectrum of NaCl varies consistently with T: at $T = 100$ K, there two peaks at 240 nm and 260 nm; while at $T = 1500$ K the peaks merge.

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[a] Yurchenko *et al* Comput Phys Commun 2016 **202** 262–275;Yurchenko *et al* A&A 2018 **614** A131

[b] Dishoeck *et al* J. Chem. Phys. 1982 **77** 3693

[c] Yang *et al* J Quant Spectrosc Radiat Transf 2020 **254** 107203